ISSN 1062-8738, Bulletin of the Russian Academy of Sciences. Physics, 2014, Vol. 78, No. 12, pp. 1265–1268. © Allerton Press, Inc., 2014.
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Electromagnetic Solitons Propagating along Quantum Wires

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Abstract—The behavior of electromagnetic pulses passing through semiconducting quantum wires is studied. An effective system of equations for the vector and scalar potential components is obtained.

DOI: 10.3103/S1062873814120168

INTRODUCTION

Advances in semiconductor technologies have allowed the growth of new structures that have unique properties and attract special attention from both theorists and experimenters. In addition to the familiar carbon nanotubes (CNTs) [1–3], which have both semiconducting and metallic properties and are typical example of one-dimensional structures, so-called whiskers have also gained popularity [4–6]. The latter can exhibit either semiconducting or metallic properties, depending on their material and method of fabrication. Numerous papers have been devoted to theoretically describing such structures, and considerable progress has been made in understanding not only their properties but the optical properties of low-dimensional materials as well. Note that the greatest development in studying optical properties has been in plasmonics, which focuses on the spectral features of low-dimensional systems [7]. Despite the results already achieved, studies of the interaction between electromagnetic fields and low-dimensional structures has mainly been limited to linear analysis, in which a field is considered to be weak. Truly nonlinear effects have been considered only in a few cases, either numerically or using the theory of perturbations. Some progress has nevertheless been made in studying the interaction between extremely short optical pulses and carbon nanotubes [8–11], for which the self-consistent problem of limiting pulse propagation in carbon nanotubes has been resolved. Here, the pulse propagated perpendicular to the nanotube axis, and the electric field was homogeneous through the nanotube. Note that the physically attractive situation in which the field propagates inhomogeneously along the nanotube axis has yet to be considered. The main difference between this situation and the ones above is that the current is also inhomogeneous, due to the field's inhomogeneity along the axis, and there is charging that induces a complementary field. We should therefore study the behavior of extremely short optical pulses in quasi-one-dimensional semiconducting structures when the pulse propagates along the structure's axis.

BASIC EQUATIONS

A nano-object's electron structure is normally studied within the strong-coupling approximation. The dispersion law describing the properties of (m, 0) CNTs has the form [12]

$$\vec{E}(\vec{p}) = \pm\gamma\sqrt{1 + 4\cos(ap_x)\cos\left(\frac{\pi s}{m}\right) + 4\cos^2\left(\frac{\pi s}{m}\right)}, \quad (1)$$

where $s = 1,2\ldots m$, $\gamma \approx 2.7$ eV, $a = 3b/2\hbar$, and $b = 0.142$ nm is the distance between neighboring carbon atoms.

To construct a model of ultrashort optical pulse propagation in a quasi-one-dimensional structure using the geometry in Fig. 1, we describe the elec-

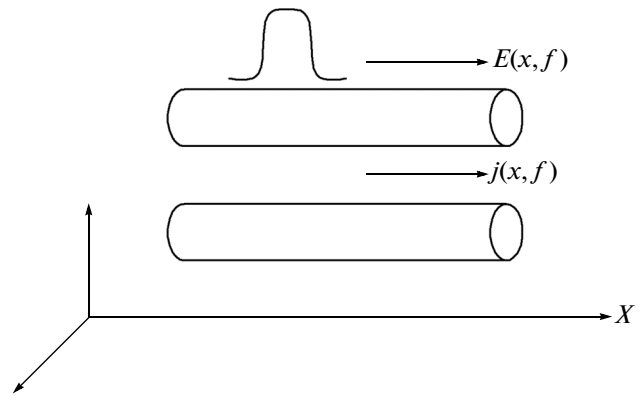

Fig. 1. Geometry of a problem where $j(x, t)$ is the current along a CNT axis and $E(x, t)$ is the electric field of the pulse.

tromagnetic field of a pulse using Maxwell's equation [13],

$$\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} - \text{grad}\varphi. \quad (2)$$

The vector potential determines the field of the extremely short pulse and has the form $\vec{A} = (A(x,t),0,0)$.

The vector potential's behavior is therefore described by Maxwell's equation

$$\frac{\partial^2 \vec{A}}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 \vec{A}}{\partial t^2} + \frac{4\pi}{c}\vec{j} = 0, \quad (3)$$

where j is the current resulting from the effect the pulse's electric field has on the electrons over the minimum conductive band of our structure. The speed of light is then considered to be 1. Here, we ignore diffraction laser beam spreading in directions perpendicular to the axis of propagation. The electric field perpendicular to the structure's axis is also not considered, since it does not contribute to the electron motion. In this model, its use does not allow interband transitions; otherwise, the laser pulse's far-IR frequency would be limited. Inasmuch as the typical size of the one-dimensional structures and the distance between them is much less than the typical size of the spatial area in which an extremely short pulse is found, we can use a continuum approximation and consider the current to be distributed over the volume.

Since we may assume that the characteristic relaxation time for electrons in semiconductors is 3×10^{-13} s [14], the ensemble of electrons at the times typical of extremely short optical pulses (on the order of 10^{-14} s) can therefore be described using the collisionless Boltzmann kinetic equation [15]

$$\frac{\partial f}{\partial t} + qE\frac{\partial f}{\partial p} = 0, \quad (4)$$

where $f = f(p_s, s, t)$ is a coordinate-implicit distribution function, and the f distribution function at the initial time is close to Fermi's equilibrium distribution function F_0:

$$F_0 = \frac{1}{1 + \exp(E(\vec{p})/k_B T)},$$

where T is temperature and k_B is the Boltzmann constant. Here, we need to make one more approximation, in which the electric field typically created by an extremely short pulse considerably exceeds the one generated by the redistribution of charge in the one-dimensional structure. The change in the electron distribution function resulting from the pulses is thus greater than the one over the coordinates.

The following expression is valid for current density $\vec{j} = (j,0,0)$:

$$j = \frac{q}{\pi\hbar}\sum_s \int \upsilon f dp, \quad (5)$$

where we introduce group velocity $\vec{\upsilon} = \partial E(\vec{p})/\partial p$.

Solving Eq. (4) via the standard method in [16], we obtain

$$j = \frac{q}{\pi\hbar}\sum_s \int_{-q_0}^{q_0} dp\upsilon\left[p + \int_{-\infty}^{t} E(t')dt'\right]F_0(\vec{p}), \quad (6)$$

Integration in (6) is performed over the first Brillouin zone, and $q_0 = \frac{2\pi\hbar}{a}$.

Equation (3) with allowance for (6) must be supplemented with a scalar φ-potential equation. The field inhomogeneity along the Ox axis redistributes the electric charge density. Inasmuch as the total charge over the sample volume is constant, the variation in charge density is determined by the continuity equation [13]

$$\frac{\partial j}{\partial x} + \frac{\partial \rho}{\partial t} = 0, \quad (7)$$

where ρ is the bulk charge density. Equation (7) enables us to establish the relation between the current and the scalar potential, keeping in mind that the scalar potential is determined by the Laplace equation

$$\frac{\partial^2 \varphi}{\partial t^2} - \frac{\partial^2 \varphi}{\partial x^2} = \beta(\rho - \rho_0), \quad (8)$$

where ρ_0 is the equilibrium charge density and $\beta = \frac{\hbar}{\varepsilon\gamma_0 a}$. Introducing the dimensionless factor, we finally obtain the system of Eqs. (9), (11), and (12):

$$\frac{\partial^2 \Phi}{\partial \tau^2} - \frac{\partial^2 \Phi}{\partial \xi^2} + \eta\sum_{s=1}^{m} G_s \sin\left(s\left(\Phi + \int_0^{\tau}\frac{\partial \Psi}{\partial \xi}d\tau\right)\right) = 0, \quad (9)$$

where $\Phi = Aea/c\hbar$ is the projection of dimensionless vector potential onto the Ox axis; $\psi = \varphi ea/\hbar$, $\tau = \omega_0 t/\sqrt{\varepsilon}$ is the dimensionless time; $\xi = \omega_0 x$ is a dimensionless coordinate; $\eta = \rho/\rho_0$, ρ_0 is the equilibrium electron concentration when there is no electromagnetic field; and ω_0 is the frequency–length magnitude determined by the formula

$$\omega_0 = 2\frac{|e|a}{\hbar}\sqrt{\pi\rho_0\gamma_0}. \quad (10)$$

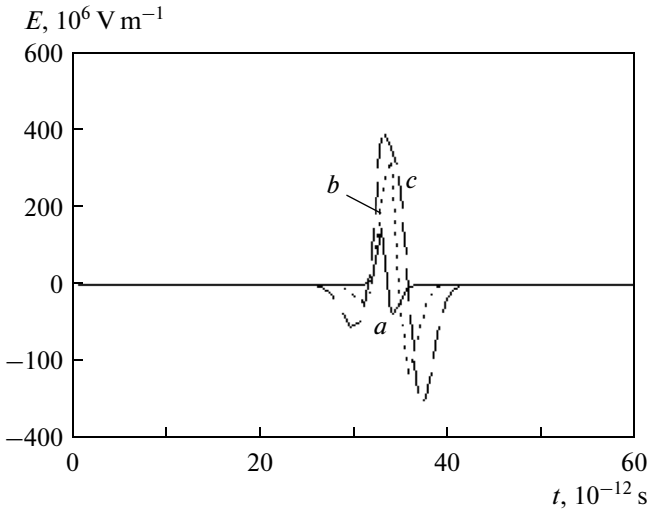

Fig. 2. Time dependences of electric field intensity ψ for different points in space: (*a*) $x = 0.5 \times 10^{-5}$ m; (*b*) $x = 2.0 \times 10^{-5}$ m; (*c*) $x = 3.0 \times 10^{-5}$ m ($Q = 0.2$).

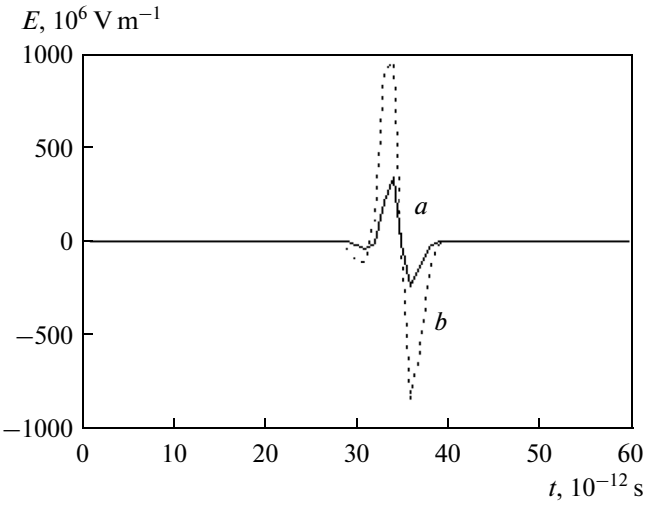

Fig. 3. Time dependence of electric field intensity ψ for different values of the initial pulse amplitude ($x = 2.0 \times 10^{-5}$ m): (*a*) $Q = 0.2$; (*b*) $Q = 1.0$.

The equation determining the variation in electron concentration in the pulse's electromagnetic field has the form

$$\frac{\partial \eta}{\partial \tau} = \alpha \sum_{s=1}^{m} G_s \frac{\partial}{\partial \xi}\left[\eta \sin\left(s\left(\Phi + \int_0^{\tau} \frac{\partial \Psi}{\partial \xi} d\tau\right)\right)\right], \qquad (11)$$

$$\alpha = \frac{\gamma_0 d}{\hbar}\sqrt{\varepsilon}.$$

The variation in scalar potential is determined by the expression

$$\frac{\partial^2 \psi}{\partial \tau^2} - \frac{\partial^2 \psi}{\partial \xi^2} = \beta(\eta - 1). \qquad (12)$$

The electric field in the nanotube bundle has the form $\mathbf{E}\{E, 0, 0\}$

$$E = -\frac{\partial A}{\partial t} = E_0 \frac{\partial \Phi}{\partial t}, \qquad (13)$$

where E_0 is determined by the formula

$$E_0 = -\frac{\hbar \omega_0}{ea\sqrt{\varepsilon}}. \qquad (14)$$

As is well known, the physical magnitude measured experimentally is the intensity of electromagnetic irradiation and is proportional to the squared module of the electric field vector [17]. The magnitude proportional to field intensity $I = |E|^2$ and governed by formula (13) is thus defined as

$$I = I_0\left(\frac{\partial \Phi}{\partial \tau}\right)^2, \quad I_0 = E_0^2. \qquad (15)$$

RESULTS FROM NUMERICAL MODELING

The system of Eqs. (9), (11), and (12) have no generally exact analytical solution, so the propagation of electromagnetic pulses in a one-dimensional structure was studied by means of numerical modeling:

We assume that a breather-like electromagnetic pulse is generated in a CNT at moment $\tau = 0$, and the nonzero component of the dimensionless vector field potential has the form

$$\Phi(\xi, \tau) = \exp\left(-\left(\frac{\xi - \xi_0}{\lambda}\right)^2\right), \qquad (16)$$

where ξ_0 denotes the dimensionless pulse coordinates along the *Ox* axis at moment $\tau = 0$, and λ is the dimensionless pulse half-width along the *Ox* axis.

We also assume that at moment $\tau = 0$, the electron concentration n in the CNT is n_0, and that scalar potential Φ is zero; i.e., we have the initial conditions $\eta(\xi, \tau) = 1$ and $\psi(\xi, \tau) = 0$.

Laser pulse propagation in an array of $(m, 0)$ carbon nanotubes was studied with the following parameters: $m = 7$, $\gamma_0 = 2.7$ eV, $b = 1.42 \times 10^{-8}$ cm, $n_0 = 2 \times 10^{18}$ cm^{-3} [14], $T = 77$ K, $\varepsilon = 4$, and $\omega_0 \approx 10^{14}$ s^{-1} (see (7)).

The evolution of an extremely short pulse is shown in Fig. 2.

The main result is that the pulse can propagate along the CNT while maintaining its shape. This is explained mathematically by our effective equation being close to the sin-Gordon equation, which allows for solitons. Physically, it is due to the balanced dispersion and nonlinearity in our effective solutions.

The shape of a pulse of an electromagnetic field as a function of the initial pulse amplitude is shown in Fig. 3.

CONCLUSIONS

The obtained dependences confirm that the stability of a pulse's shape is due to the nonlinear response of a CNT to an applied electric field. Note that the stable shape of a pulse varies with its amplitude, which is also associated with the nonlinearity of the response.

Extremely short optical pulses can thus propagate along carbon nanotubes. This in turn provides new opportunities for studying the nonlinear characteristics of both pure CNTs and CNTs with impurities.

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Translated by O. Maslova